List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Molecular-level insights on the reactive facet of carbon nitride single crystals photocatalysing overall water splitting. Nature Catalysis, 2020, 3, 649-655.	16.1	427
2	Heteroatom Dopants Promote Twoâ€Electron O ₂ Reduction for Photocatalytic Production of H ₂ O ₂ on Polymeric Carbon Nitride. Angewandte Chemie - International Edition, 2020, 59, 16209-16217.	7.2	270
3	Copolymerization with 2,4,6-Triaminopyrimidine for the Rolling-up the Layer Structure, Tunable Electronic Properties, and Photocatalysis of g-C ₃ N ₄ . ACS Applied Materials & Interfaces, 2015, 7, 5497-5505.	4.0	264
4	Carbon Vacancies in a Melon Polymeric Matrix Promote Photocatalytic Carbon Dioxide Conversion. Angewandte Chemie - International Edition, 2019, 58, 1134-1137.	7.2	208
5	CRISPR-Cas12a-Derived Photoelectrochemical Biosensor for Point-Of-Care Diagnosis of Nucleic Acid. Analytical Chemistry, 2022, 94, 7442-7448.	3.2	196
6	A Theoretical Study on the Electronic Structures of TiO2:Â Effect of Hartreeâ^'Fock Exchange. Journal of Physical Chemistry B, 2005, 109, 19270-19277.	1.2	135
7	Fully Condensed Poly (Triazine Imide) Crystals: Extended π onjugation and Structural Defects for Overall Water Splitting. Angewandte Chemie - International Edition, 2022, 61, .	7.2	114
8	An Ancient Fingerprint Indicates the Common Ancestry of Rossmann-Fold Enzymes Utilizing Different Ribose-Based Cofactors. PLoS Biology, 2016, 14, e1002396.	2.6	85
9	A Refined MS-EVB Model for Proton Transport in Aqueous Environments. Journal of Physical Chemistry B, 2012, 116, 343-352.	1.2	79
10	Heterogeneous photoredox flow chemistry for the scalable organosynthesis of fine chemicals. Nature Communications, 2020, 11, 1239.	5.8	75
11	Switching on Supramolecular Catalysis via Cavity Mediation and Electrostatic Regulation. Angewandte Chemie - International Edition, 2016, 55, 12778-12782.	7.2	64
12	Mechanisms of Hydrogen-Assisted CO ₂ Reduction on Nickel. Journal of the American Chemical Society, 2017, 139, 4663-4666.	6.6	63
13	Heteroatom Dopants Promote Twoâ€Electron O ₂ Reduction for Photocatalytic Production of H ₂ O ₂ on Polymeric Carbon Nitride. Angewandte Chemie, 2020, 132, 16343-16351.	1.6	59
14	Interfacial engineering of lattice coherency at ZnO-ZnS photocatalytic heterojunctions. Chem Catalysis, 2022, 2, 125-139.	2.9	56
15	Negative Ion Photoelectron Spectroscopy Reveals Thermodynamic Advantage of Organic Acids in Facilitating Formation of Bisulfate Ion Clusters: Atmospheric Implications. Journal of Physical Chemistry Letters, 2013, 4, 779-785.	2.1	53
16	Density Functional Theory Study of Single-Atom V, Nb, and Ta Catalysts on Graphene and Carbon Nitride for Selective Nitrogen Reduction. ACS Applied Nano Materials, 2020, 3, 5149-5159.	2.4	51
17	Whether Corrugated or Planar Vacancy Graphene-like Carbon Nitride (g-C ₃ N ₄) Is More Effective for Nitrogen Reduction Reaction?. Journal of Physical Chemistry C, 2019, 123, 17296-17305.	1.5	46
18	High photoluminescent carbon based dots with tunable emission color from orange to green. Nanoscale, 2017, 9, 1028-1032.	2.8	43

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19	Well-defined Co ₉ S ₈ cages enable the separation of photoexcited charges to promote visible-light CO ₂ reduction. Nanoscale, 2021, 13, 18070-18076.	2.8	43
20	Carbon Vacancies in a Melon Polymeric Matrix Promote Photocatalytic Carbon Dioxide Conversion. Angewandte Chemie, 2019, 131, 1146-1149.	1.6	42
21	Global triplet potential energy surfaces for the N2(<i>X</i> 1Σ) + O(3 <i>P</i>) → NO(<i>X</i> 2Î) + N(4 <i>S</i>) reaction. Journal of Chemical Physics, 2016, 144, 024309.	1.2	41
22	Highly Active and Sulfurâ€Resistant Fe–N ₄ Sites in Porous Carbon Nitride for the Oxidation of H ₂ S into Elemental Sulfur. Small, 2020, 16, e2003904.	5.2	41
23	Remarkable oxygen evolution by Co-doped ZnO nanorods and visible light. Applied Catalysis B: Environmental, 2021, 296, 120369.	10.8	38
24	Hydrogenation of CO to Methanol on Ni(110) through Subsurface Hydrogen. Journal of the American Chemical Society, 2017, 139, 17582-17589.	6.6	35
25	What Is the Best Size of Subnanometer Copper Clusters for CO ₂ Conversion to Methanol at Cu/TiO ₂ Interfaces? A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 24118-24132.	1.5	32
26	Relative Efficacy of Coâ^'X ₄ Embedded Graphene (X=N, S, B, and P) Electrocatalysts towards Hydrogen Evolution Reaction: Is Nitrogen Really the Best Choice?. ChemCatChem, 2020, 12, 536-543.	1.8	32
27	Unraveling the mechanisms of S-doped carbon nitride for photocatalytic oxygen reduction to H ₂ O ₂ . Physical Chemistry Chemical Physics, 2020, 22, 21099-21107.	1.3	29
28	Effects of doping high-valence transition metal (V, Nb and Zr) ions on the structure and electrochemical performance of LIB cathode material LiNi _{0.8} Co _{0.1} Mn _{0.1} O ₂ . Physical Chemistry Chemical Physics, 2021, 23, 11528-11537.	1.3	29
29	Blue-AsP monolayer as a promising anode material for lithium- and sodium-ion batteries: a DFT study. Physical Chemistry Chemical Physics, 2021, 23, 5143-5151.	1.3	28
30	Electrocatalytic Nitrogen Reduction by Transition Metal Single-Atom Catalysts on Polymeric Carbon Nitride. Journal of Physical Chemistry C, 2021, 125, 13880-13888.	1.5	28
31	Structural characterizations and electronic properties of Ti-doped SnO2(110) surface: A first-principles study. Journal of Chemical Physics, 2006, 124, 054704.	1.2	27
32	Effects of Surface Pressure on the Properties of Langmuir Monolayers and Interfacial Water at the Air–Water Interface. Langmuir, 2015, 31, 2147-2156.	1.6	27
33	<i>Ab initio</i> quantum dynamics of charge carriers in graphitic carbon nitride nanosheets. Journal of Chemical Physics, 2020, 153, 054701.	1.2	27
34	Fast and Slow Proton Transfer in Ice: The Role of the Quasi-Liquid Layer and Hydrogen-Bond Network. Journal of Physical Chemistry B, 2014, 118, 8081-8089.	1.2	26
35	Reducing CO ₂ to CO and H ₂ O on Ni(110): The Influence of Subsurface Hydrogen. Journal of Physical Chemistry C, 2016, 120, 23061-23068.	1.5	26
36	Nitrogen fixation on metal-free SiC(111) polar surfaces. Journal of Materials Chemistry A, 2020, 8, 7412-7421.	5.2	26

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37	Switching on Supramolecular Catalysis via Cavity Mediation and Electrostatic Regulation. Angewandte Chemie, 2016, 128, 12970-12974.	1.6	24
38	High-performance potassium poly(heptazine imide) films for photoelectrochemical water splitting. Chemical Science, 2022, 13, 7541-7551.	3.7	24
39	A quasiclassical trajectory study of the N2(X1Σ) + O(3P) → NO(X2Î) + N(4S) reaction. Journal of Chemical Physics, 2016, 144, 234314.	1.2	23
40	A New Candidate in Polyanionic Compounds for a Potassium-Ion Battery Cathode: KTiOPO ₄ . Journal of Physical Chemistry Letters, 2021, 12, 2721-2726.	2.1	23
41	Chemisorption of OCN on Cu (100) surface: a density functional study. Journal of Solid State Chemistry, 2004, 177, 2763-2771.	1.4	22
42	BC ₂ N/Graphene Heterostructure as a Promising Anode Material for Rechargeable Li-Ion Batteries by Density Functional Calculations. Journal of Physical Chemistry C, 2019, 123, 30809-30818.	1.5	22
43	Highly Poisonâ€Resistant Singleâ€Atom Co–N ₄ Active Sites with Superior Operational Stability over 460Âh for H ₂ S Catalytic Oxidation. Small, 2021, 17, e2104939.	5.2	21
44	A boron-decorated melon-based carbon nitride as a metal-free photocatalyst for N ₂ fixation: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 21872-21880.	1.3	18
45	Improving the C _β Stereoselectivity of <scp>l</scp> â€Threonine Aldolase for the Synthesis of <scp>lâ€</scp> <i>threo</i> â€4â€Methylsulfonylphenylserine by Modulating the Substrateâ€Binding Pocket To Control the Orientation of the Substrate Entrance. Chemistry - A European Journal, 2021, 27, 9654-9660	1.7	17
46	Systematic Study of Structural and Thermodynamic Properties of HCl(H ₂ 0) _{<i>n</i>} Clusters from Semiempirical Replica Exchange Simulations. Journal of Physical Chemistry A, 2013, 117, 7131-7141.	1.1	15
47	Direct Observation of Hierarchic Molecular Interactions Critical to Biogenic Aerosol Formation. Communications Chemistry, 2018, 1, .	2.0	15
48	Exploring the potentials of Ti ₃ N ₂ and Ti ₃ N ₂ X ₂ (X = O, F, OH) monolayers as anodes for Li or non-Li ion batteries from first-principles calculations. RSC Advances, 2019, 9, 40340-40347.	1.7	15
49	Defective BC ₂ N as an Anode Material with Improved Performance for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 4946-4954.	1.5	15
50	Improvement of photocatalytic activity of g-C3N4 by five-membered heterocyclic small molecule modifications: A theoretical prediction. Applied Surface Science, 2019, 478, 119-127.	3.1	14
51	Fluorescent Se-modified carbon nitride nanosheets as biomimetic catalases for free-radical scavenging. Chemical Communications, 2020, 56, 916-919.	2.2	14
52	Fully Condensed Poly (Triazine Imide) Crystals: Extended Ï€â€Conjugation and Structural Defects for Overall Water Splitting. Angewandte Chemie, 2022, 134, .	1.6	14
53	Atomistic Observation of Temperature-Dependent Defect Evolution within Sub-stoichiometric WO _{3–<i>x</i>} Catalysts. ACS Applied Materials & Interfaces, 2022, 14, 2194-2201.	4.0	14
54	Investigating Single-Molecule Fluorescence Spectral Heterogeneity of Rhodamines Using High-Throughput Single-Molecule Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 3914-3921.	2.1	12

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55	Infrared Spectra of HCl(H ₂ O) _{<i>n</i>} Clusters from Semiempirical Born–Oppenheimer Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2015, 119, 4450-4456.	1.1	11
56	Stimuli-responsive metal–organic supercontainers as synthetic proton receptors. Dalton Transactions, 2018, 47, 10256-10263.	1.6	11
57	Investigation of Ordered TiMC and TiMCT ₂ (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries. Journal of Physical Chemistry C, 2022, 126, 5283-5291.	1.5	9
58	Construction of an Efficient Non-natural Enzyme System for Preparation of Testosterone in High Space-Time Yield. ACS Sustainable Chemistry and Engineering, 2022, 10, 3373-3382.	3.2	7
59	Effects of Ti doping at the reduced SnO2(110) surface with different oxygen vacancies: a first principles study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	6
60	Mechanisms of Formaldehyde and C ₂ Formation from Methylene Reacting with CO ₂ Adsorbed on Ni(110). Journal of Physical Chemistry C, 2018, 122, 13827-13833.	1.5	6
61	Molecular-Level Insight into the Hydroxylated Monomeric VO _{<i>x</i>} /Î,-Al ₂ O ₃ (010) and Its Adsorption of Methanol. Journal of Physical Chemistry C, 2019, 123, 27704-27711.	1.5	6
62	The sources of hydrogen affect the productivity and selectivity of CO2 photoreduction on SiC. Applied Surface Science, 2021, 538, 148010.	3.1	6
63	Theoretical insights into the thermal reduction of N2 to NH3 over a single metal atom incorporated nitrogen-doped graphene. Journal of Chemical Physics, 2021, 154, 054703.	1.2	6
64	Unveiling the Selectivity of CO ₂ Reduction on Cu ₂ ZnSnS ₄ : The Effect of Exposed Termination. Journal of Physical Chemistry C, 2021, 125, 24967-24973.	1.5	6
65	Validation of Density Functional Theory Methods for Predicting the Optical Properties of Cu-Based Multinary Chalcogenide Semiconductors. Journal of Physical Chemistry C, 2022, 126, 4684-4697.	1.5	6
66	DFT investigations of KTiOPO4M <i>x</i> (M = K, Na, and Li) anodes for alkali-ion battery. Journal of Chemical Physics, 2022, 156, .	1.2	6
67	Microscopic functionality of FeN4 sites in polymeric carbon nitride for efficient H2S oxidation. Applied Surface Science, 2022, 600, 154011.	3.1	6
68	Understanding the Role of Various Dopant Metals (Sb, Sn, Ga, Ge, and V) in the Structural and Electrochemical Performances of LiNi _{0.5} Co _{0.2} Mn _{0.3} O ₂ . Journal of Physical Chemistry C 2021 125 19600-19608	1.5	5
69	Antifreeze protein NMR sensor to detect water molecular reorientation in the surface of ice. Journal of Chemical Physics, 2009, 131, .	1.2	4
70	An Organic Molecular Photocatalyst Releasing Oxygen from Water. ChemSusChem, 2019, 12, 4854-4858.	3.6	4
71	Theoretical Insights into Synergistic Effects at Cu/TiC Interfaces for Promoting CO2 Activation. ACS Omega, 2021, 6, 27259-27270.	1.6	4
72	How does the defect ZnO@Au surface activate the methane via the precursor-mediated mechanism?. Applied Surface Science, 2021, 555, 149728.	3.1	3

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73	Facile fabrication of oxygen-doped carbon nitride with enhanced visible-light photocatalytic degradation of methyl mercaptan. Research on Chemical Intermediates, 2022, 48, 2295-2311.	1.3	3
74	Hydrogenation of CO on Ni(110) by Energetic Deuterium. Journal of Physical Chemistry C, 2018, 122, 14671-14677.	1.5	2
75	Submonolayer Is Enough: Switching Reaction Channels on Pt/SiO2 by Atomic Layer Deposition. Journal of Physical Chemistry C, 2021, 125, 18725-18733.	1.5	2